

IN THE CLAIMS:

The text of all pending claims (including withdrawn claims) is set forth below. Cancelled and not entered claims are indicated with claim number and status only. The claims as listed below show added text with underlining and deleted text with ~~strikethrough~~. The status of each claim is indicated with one of (original), (currently amended), (cancelled), (withdrawn), (new), (previously presented), or (not entered).

Please AMEND claims 16, 17, and 23-25 in accordance with the following:

1-15. (Cancelled)

16. (Currently Amended) A method of determining spatially similar portions of substances by analyzing three-dimensional structures of ~~the a substances substance~~ including by comparing a first probe structure expressed by three-dimensional coordinates of elements belonging to a first subset of a plurality of subsets of secondary structures of probe structures, the first subset comprising a first point set of an amino acid sequence database or a motif database and a second target structure expressed by three-dimensional coordinates of elements belonging to a second subset of a plurality of subsets of secondary structures of the target structure, the second subset comprising a second point set of an input amino acid sequence of the target structure, comprising:

dividing the second structure into a plurality of second subsets based on secondary structures of the three-dimensional coordinates of the target structure;

~~dividing the first point set and second point set into first subsets and second subsets, respectively, according to a secondary structure exhibited by the three-dimensional coordinates of the elements of the first and the second point sets;~~

determining whether a correspondence is present between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure by, for each subset of the plurality of subsets of secondary structures of the target structure:

_____ generating a first tree structure for the first point set of the probe structure and a second tree structure for the second point set of the target structure;

_____ pruning the second tree structure for the second point set of the plurality of second subsets of the target structure in accordance with a predetermined pruning procedure;
and

_____ determining whether the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, and if the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, generating a correspondence between

the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; and

~~—generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;~~

~~determining the optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of correspondence generated; and~~

~~calculating a root mean square distance (RMSD) between all of the elements corresponding in the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure the optimum correspondence to automatically determine a distance between the elements of the first point set and the elements of the second point set;~~

~~determining whether the RMSD is less than or equal to a predetermined threshold value, and where the RMSD is less than or equal to a predetermined threshold value, generating an optimum correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; that have an optimal~~
~~correspondence and~~

~~to determined~~determining a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence having a ~~greatest~~the optimum correspondence to the input amino acid sequence.

17. (Currently Amended) The method of claim 16, wherein determining the optimum correspondence the length of a longest common subsequence comprises:

~~generating a combination of correspondence satisfying a second restriction condition between the elements belonging to the subsets corresponding in the combination of the correspondence generated;~~

~~—calculating a root mean square distance between the elements corresponding in the combination of the correspondence generated satisfying the second restriction condition; and~~

~~selecting a combination of the correspondence as the optimum correspondence according to the value of the root mean square distance value calculated to determine the LCS and an occurrence position of the LCS between the~~

selecting a character sequence expressing the input amino acid sequence of the target structure and the that has the optimum correspondence with a character sequence of the probe structure having the greatest correspondence and expressing an amino acid sequence taken from the amino acid sequence database or the motif database, and

_____ aligning the character sequence of the input amino acid sequence of the target structure with the character sequence of the probe structure having the greatest optimum correspondence to determine the LCS and an occurrence position of the LCS, and
_____ expressing the amino acid sequence from the amino acid sequence database or the motif database, based on the LCS and the occurrence position of the LCS, by inserting a blank corresponding to a length of a character sequence between positions of subsequences.

18-22. (Cancelled)

23. (Currently Amended) An apparatus for determining spatially similar portions of substances by analyzing three-dimensional structures of ~~the a substances substance including by~~ comparing a first probe structure expressed by three-dimensional coordinates of elements belonging to a first subset of a plurality of subsets of secondary structures of probe structures, the first subset comprising a first point set of an amino acid sequence database or a motif database and a second target structure expressed by three-dimensional coordinates of elements belonging to a second subset of a plurality of subsets of secondary structures of the target structure, the second subset comprising a second point set of an input amino acid sequence of the target structure, comprising:

a dividing unit to divide the second structure into a plurality of second subsets based on secondary structures of the three-dimensional coordinates of the target structure;

~~a dividing unit to divide the first point set and the second point set into first subsets and second subsets, respectively, according to a secondary structure exhibited by the three-dimensional coordinates of the elements of the first and the second point sets;~~

~~a generating unit to generate a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;~~

a determining unit to determine whether a correspondence is present between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure by, for each subset of the plurality of subsets of secondary structures of the target structure:

generating a first tree structure for the first point set of the probe structure and a second tree structure for the second point set of the target structure;

pruning the second tree structure for the second point set of the plurality of second subsets of the target structure in accordance with a predetermined pruning procedure;
and

determining whether the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, and if

the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, generating a correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; and

~~determine an optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of correspondence generated in the generating unit, and~~
a calculating unit to

calculate a root mean square distance (RMSD) between all of the elements corresponding in the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure ~~the optimum correspondence~~, to automatically determine a distance between the elements of the first point set and the elements of the second point set;

determine whether the RMSD is less than or equal to a predetermined threshold value, and where the RMSD is less than or equal to a predetermined threshold value, generating an optimum correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; that have an optimal correspondence and

~~to~~ determine a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence having a ~~greatest~~ optimum correspondence to the input amino acid sequence.

24. (Currently Amended) A computer-readable medium containing computer-readable instructions to determine spatially similar portions of substances by analyzing three-dimensional structures of ~~the a substances~~ substance including by comparing a first probe structure expressed by three-dimensional coordinates of elements belonging to a first subset of a plurality of subsets of secondary structures of probe structures, the first subset comprising a first point set of an amino acid sequence database or a motif database and a second target structure expressed by three-dimensional coordinates of elements belonging to a second subset of a plurality of subsets of secondary structures of the target structure, the second subset comprising a second point set of an input amino acid sequence of the target structure, the computer-readable instructions comprising:

~~dividing the first point set expressing a position of an amino acid of the amino acid sequence taken from the amino acid sequence database or the motif database and second point set expressing a position of an amino acid of the input amino acid sequence into a~~

~~plurality of first subsets and second subsets, respectively,~~ according to a secondary structure of the target structure exhibited by the three-dimensional coordinates of the elements of ~~the first and the second point sets~~set;

determining whether a correspondence is present between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure by, for each subset of the plurality of subsets of secondary structures of the target structure:

generating a first tree structure for the first point set of the probe structure and a second tree structure for the second point set of the target structure;

pruning the second tree structure for the second point set of the plurality of second subsets of the target structure in accordance with a predetermined pruning procedure;
and

determining whether the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, and if the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, generating a correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; and

~~—generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;~~

~~—determining the optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of correspondence generated; and~~

calculating a root mean square distance (RMSD) between all of the elements corresponding in the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure in the optimum correspondence, to automatically determining-determine a distance between the elements of the first point set and the elements of the second point set;

determining whether the RMSD is less than or equal to a predetermined threshold value, and where the RMSD is less than or equal to a predetermined threshold value, generating an optimum correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; that have an optimal correspondence and and

determining a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence having a-greatestthe optimum correspondence to the input amino acid

sequence.

25. (Currently Amended) The computer-readable medium of claim 24, wherein determining the length of a longest common subsequence ~~the optimum correspondence~~ comprises:

~~—generating a combination of correspondence satisfying a second restriction condition between the elements belonging to the subsets corresponding in the combination of the correspondence generated;~~

~~—calculating a root mean square distance between the elements corresponding in the combination of the correspondence generated satisfying the second restriction condition; and~~

~~—selecting a combination of the correspondence as the optimum correspondence according to the value of the root mean square distance value calculated, determining the LCS and an occurrence position of the LCS between the~~

selecting a character sequence expressing the input amino acid sequence of the target structure and the that has the optimum correspondence with a character sequence of the probe structure ~~having the greatest correspondence and expressing an amino acid sequence taken from the amino acid sequence database or the motif database, and~~

aligning the character sequence of the input amino acid sequence of the target structure with the character sequence of the probe structure having the greatest optimum correspondence to determine the LCS and an occurrence position of the LCS, and

expressing the amino acid sequence from the amino acid sequence database or the motif database, based on the LCS and the occurrence position of the LCS, by inserting a blank corresponding to a length of a character sequence between positions of subsequences.

26. (Withdrawn) A computer-readable medium containing computer-readable instructions to compare spatially similar portions of an input amino acid sequence and an amino acid sequence taken from an amino acid sequence database or a motif database, the computer-readable instructions comprising:

searching the amino acid sequence database and the motif database for an amino acid sequence or sequences having at least a predetermined degree of similarity to the input amino acid sequence;

determining a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence having a greatest degree of similarity to the input amino acid sequence, wherein the amino acid sequence having the greatest degree of similarity is selected from a set of amino acid sequences having at least the predetermined degree of similarity;

determining the LCS and an occurrence position of the LCS between the character sequence expressing the input amino acid sequence and the character sequence having the greatest degree of similarity and expressing an amino acid sequence taken from the amino acid sequence database or the motif database; and

aligning the character sequence of the input amino acid sequence with the character sequence having the greatest degree of similarity and expressing the amino acid sequence from the amino acid sequence database or the motif database, based on the LCS and the occurrence position of the LCS, by inserting a blank corresponding to a length of a character sequence between positions of subsequences.